ESCM2002

Electronic Structure and Computational Magnetism

15-17 July 2002

Georgetown University
Washington, DC, U.S.A.

Welcome to Washington.

PROGRAM

ESCM2002: Electronic Structure and Computational Magnetism

Georgetown University
Washington, DC, U.S.A.

SUNDAY, JULY 14, 2002

17:00-19:00	Registration and Welcoming Reception	Physics Department

MONDAY, JULY 15, 2002

08:30-08:40	Welcome	
Session 1	**G.M. Stocks, Chair**	
08:40-09:15	G. Kotliar	Correlation Effects in Magnetic Properties: A First Principles Dynamical Mean Field Approach
09:15-09:50	R. de Groot	Spin-Injection from Half-Metals
09:50-10:10	W. Ku	Wannier State Analysis of Insulating Ferromagnetism in $La_4Ba_2Cu_2O_{10}$
10:10-10:30	**Coffee**	
Session 2	**D.D. Koelling, Chair**	
10:30-11:05	M. Troyer	Exchange Couplings in Cuprates and Vanadates from QMC and Ab-Initio Calculations
11:05-11:25	N. Kioussis	Phase Diagram of the Symmetric and Asymmetric One-dimensional Periodic Anderson Models
11:25-12:00	S.C. Erwin	Self-Compensation in Manganese-Doped Ferromagnetic Semiconductors
12:00-12:20	P. Mahadevan	Ferromagnetism in Dilute Magnetic Semiconductors
12:20-13:45	Lunch	
Session 3	**H. Eschrig, Chair**	
13:45-14:20	W. Lambrecht	Magnetic Properties of Transition Metal Impurities in SiC
14:20-14:40	Y.-J. Zhao	Advanced Tetrahedrally-Bonded Magnetic Semiconductors for Spintronic Applications
14:40-15:15	W.H. Butler	Electronic and Magnetic Structure of a Room Temperature Magnetic Semiconductor: Ilmenite-alpha-Hematite
15:15-15:35	**Coffee**	
Session 4	**D.A. Papaconstantopoulos, Chair**	
15:35-16:10	A.I. Lichtenstein	Non-Quasiparticle States in Half-Metallic Ferromagnets
16:10-16:25	I.I. Mazin	Correlated metals and the LDA+U method
16:25-17:00	P. Blaha	Charge Distribution and EFGs in Cuprates using the LDA+U Method
17:00-17:35	M.R. Pederson	2nd and 4th-order Anisotropies in Molecular Magnets
17:35-17:50	L. Senapati	Atomic Structure, Binding Energy, and Magnetic Properties of Iron Atoms Supported on Polyaromatic Hydrocarbons
18:15-21:00	**Posters and Reception**	

POSTER PAPERS

P1	A. Aguayo and D.J. Singh	Itinerant Ferromagnetism and Quantum Criticality in Sc_3In
P2	T. Baruah and M.R. Pederson	Ab initio electronic Structure and Magnetic Anisotropy Energy of Co_4-Based Single Molecule Magnet
P3	M.R. Beltran, S. Khanna, P. Jena	Determination of Magnetic Moments at the Nanoscale: The Ni_7 Case
P4	S. Cottenier, B. De Vries, J. Meersschaut, and M. Rots	The spin-density wave in Chromium: Ground State and Impurity Hyperfine Fields
P5	M. Eisenbach, B. Ujfalussy, G. Brown, and G.M. Stocks	Magnetic Properties of Iron Nanowires on Copper
P6	H.J. Gotsis and I.I. Mazin	Ferromagnetism and Spin-Orbital Compensation in Sm Intermetallics
P7	S. V. Halilov, F. Schiller, and C. Laubschat	Magnetic Surface States in Two-Dimensional Transition-Metal-Based Compounds
P8	C.S. Hellberg	Implementing Universal Quantum Computation with the Exchange Interaction
P9	M. Lach-hab, D.A. Papaconstantopoulos, I.I. Mazin and M.J. Mehl	The effect of the exchange splitting on the magnetic anisotropy of Ni
P10	P. Larson, I.I. Mazin and D.A. Papaconstantopoulos	Large Magnetic properties of YCo_5 and $SmCo_5$
P11	O. Le Bacq, A. Pasturel, A-M Dulac and S. Jobyck	Optimized Antiferromagnetic Orthophosphates for Lithium Battery Cathodes
P12	G.K.H. Madsen, K. Schwarz, P. Blaha and D.J. Singh	Magnetic Inclusion Compounds: The Alkali-Electro Sodalites and the Rare-Earth Containing Clathrates
P13	P.M. Marcus and S.L. Qiu	Instability of bcc Ferromagnetic Fe Under Pressure
P14	O.N. Mryasov and R.F. Sabirianov	A Model of Magnetization Thermal Fluctuations in Mono-Domain FePt Particles
P15	N. Noginova, E. Arthur, G. B. Loutts and V.A. Atsarkin	Slow Jahn-Teller Dynamics and Carrier Transport In Diamagnetically Diluted Perovskite Manganites
P16	D.A. Papaconstantopoulos and C.S. Hellberg	Tight-binding v. LDA+U in FeAl
P17	A. G. Petukhov and S.C. Erwin	Spin-Spin Interactions and Ferromagnetism in Mn-Doped GaAs
P18	M. Prikhodko and W. Lambrecht	Magnetic properties of Mn-N compounds
P19	D. Saifullaeva and S. Solieva	New Magnetic Semiconductors $CuCr_{1.5}Sb_{0.5}S_4$ with $CoCr_2S_4$
P20	D.J. Singh, M. Gupta and R. Gupta	Magnetism and Electronic Structure in $ZnFe_2O_4$ and $MnFe_2O_4$
P21	G. Steinle-Neumann, L. Stixrude and R. E. Cohen	Evidence for Antiferromagnetic Correlations in HCP Iron
P22	J. M. Sullivan and S. C. Erwin	Theory of the Role of Defects in Co-doped TiO_2 Anatase

TUESDAY, JULY 16, 2002

Session 5	**I.I. Mazin, Chair**	
08:30-09:05	J. Mathon	Theory of Spin-Dependant Tunneling in Magnetic Multilayers
09:05-09:40	C. Lambert	Spin-Polarised Transport in Hybrid Ferromagnetic-Superconducting Nanostructures
09:40-10:00	D. Wortmann	Spin-Polarized Ballistic Electron Transport Through an Interface by an Embedded Green-Function Approach
10:00-10:20	A. G. Petukhov	Resonant Enhancement of Tunneling Magnetoresistance in Double-Barrier Magnetic Heterostructures
10:20-10:45	M. Stiles	Transverse Spin Currents and Torques in Magnetic Multilayers
10:45-11:05	**Coffee**	
Session 6	**W.H. Butler, Chair**	
11:05-11:40	I. Mertig	Spin-Filter Effect in Metallic Nanowires
11:40-12:15	L. Nordstrom	In-Plane Uniaxial Anisotropy at the Fe/ZnSe(001) Interface
12:15-13:45	**Lunch**	
Session 7	**B.N. Harmon, Chair**	
13:45-14:20	R.W. Chantrell	Multi-Scale Modeling of Magnetic Materials
14:20-14:55	D.P. Landau	Spin Dynamics Simulations of Excitations and Critical Dynamics in a Heisenberg Antiferromagnet
14:55-15:30	G.P. Brown	Micromagnetic Modeling at Finite Temperature
15:30-15:50	P. Visscher	Spin Wave Instabilities in Magnetic Switching
15:50-16:10	**Coffee**	
Session 8	**D.J. Singh, Chair**	
16:10-16:30	V. Dobrovitski	An Approach to Multiscale Simulations of Nonlinear Magnetization Dynamics
16:30-16:45	K. Belashchenko	Multiscale approach to hysteretic phenomena: Application to CoPt-type magnets
16:45-17:20	B. Ujfalussy	Magnetic Anisotropy in Fe Multilayers on Cu
17:20-17:55	T.C. Schulthess	On the Microscopic Origin of Exchange Bias: The Role of Anisotropic Exchange
18:00-18:45	**Reception**	
18:45-21:30	**Conference Dinner**	

WEDNESDAY, JULY 17, 2002

Session 9	**A.I. Lichtenstein, Chair**	
08:30-09:05	H. Eschrig	Versions of LSDA+U for Magnetic Structures
09:05-09:40	B. Gyorffy	Exploring dynamical magnetism with Time Dependent Density Functional Theory (TDFT):from Spin Fluctuations to Gilbert Damping
09:40-10:15	J.B. Staunton	The Onset of Magnetic Order in Fe and Co Films On and Embedded in Non-Magnetic Substrates
10:15-10:35	**Coffee**	
Session 10	**J. Serene, Chair**	
10:35-10:50	S. Savrasov	Linear Response Calculations of Lattice Dynamics in Antiferromagnetic Insulators
10:50-11:25	S. Blugel	Magnetism Under the Scanning Tunneling Microscope
11:25-12:00	H. Ebert	Influence of Spin-Orbit Coupling on the Electron Spectroscopy of Non-Magnetic Metals
12:00-12:35	V.N. Antonov	Electronic Structure, Magneto-Optical Kerr Effect and X-Ray Magnetic Dichroism in Strongly Correlated Systems
12:35-13:45	**Lunch**	
Session 11	**L. Nordstrom, Chair**	
13:45-14:20	L. Sandratskii	Parameter-Free Calculation of the Exchange Interactions in Complex Magnetic Systems
14:20-14:55	M.I. Katsnelson	Many - Body Effects at Transition Metal Surfaces: an Orbital Kondo Resonance in Chromium
14:55-15:20	V.J. Thakor	Ab-initio calculations of anisotropy in spin-fluctuations of Sr_2RuO_4 and hcp-Fe
15:20-15:35	**Coffee**	
Session 12	**S. Blugel, Chair**	
15:35-16:00	R.E. Cohen	Non-Collinear Magnetism in Iron
16:00-16:20	V.P. Antropov	Self-Consistent Version of the Many Body Green Function Approach Suitable for Transition Metals Studies
16:20-16:40	O. Le Bacq	Ab-Initio Calculation of the Magnetic Anisotropy Energy of Fe-V Multilayers
16:40	**Conference Closing**	

ABSTRACTS

Itinerant Ferromagnetism and Quantum Criticality in Sc_3In

A. Aguayo[1] and D.J. Singh
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The electronic structure and magnetic properties of hexagonal Sc_3In are calculated within density functional theory. We find that the Fermi energy lies in a region of flat Sc d derived bands leading to a peak in the density of states and Stoner ferromagnetism. The calculated local spin density and generalized gradient approximation spin magnetizations are both enhanced with respect to experiment, which is an indication of significant quantum critical fluctuations, neglected in these approximations. We find, as expected, that the ferromagnetism is initially enhanced under pressure, meaning that the critical point cannot be reached with modest pressure. However, we find that the density of states peak around the Fermi energy and the calculated density functional magnetic properties are sensitive to the c/a ratio, so that the quantum critical point may be reached under uniaxial strain.

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Electronic Structure, Magneto-Optical Kerr Effect and X-Ray Magnetic Dichroism in Strongly Correlated Systems

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The optical, magneto-optical and x-ray magnetic circular dichroism (XCMD) spectra of charge-ordered magnetite (Fe_3O_4) below the Verwey transition and Mg-, Al-, Mn-, Co-, and Ni-, substituted Fe_3O_4 are investigated theoretically from first principles, using the fully relativistic Dirac LMTO band structure method. The electronic structure is obtained with the local spin-density approximation (LSDA), the fully relativistic Dirac LMTO band structure method. The electronic structure is obtained with the local spin-density approximation (LSDA), as well as with the so-called LSDA+U approach. The origin of the Kerr rotation and XCMD realized in the compounds is examined.

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Self-Consistent Version of the Many Body Green Function Approach Suitable for Transition Metals Studies

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We present a new self-consistent version of the many body Green function approach suitable for transition metals studies, which uses the quasiparticle wave functions as a basis set without referring to LDA potential or wave functions. The distinguishing feature of our approach is the use of one-site approximation and the self-consistent quasiparticle wave function basis set obtained from the solution of the Schrodinger equation with a nonlocal potential. We analyze several sets of skeleton diagrams as generating functionals for the Green function self-energy, including GW and fluctuating exchange sets. Their relative contribution to the electronic structure in 3d-metals was identified. Calculations for Fe and Ni revealed stronger energy dependence of the effective interaction and self-energy of the d-electrons near the Fermi level compared to s and p electron states. Reasonable agreement with experimental results is obtained. The proposed technique can be naturally used for total energy calculations. In addition a new theory of exchange coupling parameters calculation which is suitable for arbitrary magnetic orderings and full-potential calculations using both density functional and many body Green function approach is proposed. The validity of old theories of exchange interactions is reviewed. The extensive calculations for transition metals magnets will be discussed. In summary we believe that our approach can be considered not only as a practical ab-initio alternative to modern DFT methods with a much wider range of applicability, but simultaneously with DFT provide a more consistent tool for studying of transition metals and their compounds.

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Ab initio electronic Structure and Magnetic Anisotropy Energy of Co_4-based single Molecule Magnet

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We present our density functional based calculation of electronic structure and magnetic anisotropy energy of $Co_4(hmp)_4(CH_3OH)_4Cl_4$ where hmp is deprotonated hydroxymethyl pyridine. The experimental measurements show a high anisotropy barrier $\sim$ 100 - 200K. We find the molecule to be in S=6 state which implies a ferromagnetic ordering in agreement with experiment. We also show that the anisotropy barrier is highly influenced by the ligand separation and that the barrier height increases for other conformers in which the the Cl anions and hmp ligands are rearranged. The origin of the uniaxial anisotropy is investigated based on local hamiltonian.

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Multiscale approach to hysteretic phenomena: Application to CoPt-type magnets

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Magnetization reversal is an inherently multiscale process controlled by the interaction of magnetic domains with microstructure. Therefore, a quantitative theory of hysteretic phenomena should be based on a combined description of (a) microstructure, (b) properties of individual defects, and (c) collective effect of defect patterns on the evolving domain structure. We discuss the methodology of such multiscale modeling including first-principles, micromagnetic and microstructural calculations. The role of ab initio calculations of defect properties and exchange constant anisotropy are emphasized along with their limitations. Using a combination of the above methods we implemented the first workable approach for the description of hysteretic phenomena in nanoscale magnets and applied it to CoPt-type alloys. We show that coercivity and magnetization reversal in these magnets are governed by two generic effects originating at different length scales: a peculiar splitting of domain walls at twin boundaries and their strong pinning at antiphase boundaries. We emphasize that such multiscale nature of hysteretic phenomena is a typical feature of nanoscale magnetic materials.

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Determination of Magnetic Moments at the Nanoscale: The Ni_7 Case

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Magnetic moments of small atomic clusters are currently determined via Stern-Gerlach experiments used to demonstrate the spin quantization in atoms. The reduction in size reduces the magnetic anisotropy of the particles and small clusters are known to be superparamagnetic. Determination of the instrinsic magnetic moment of these particles from the deflections of the Stern-Gerlach profiles is a non-trivial task since it requires a knowledge of the cluster temperature and a precise measurement of the deflection profile. The problem is particularly acute for small clusters since the intrinsic cluster moments are not sufficiently large to result in appreciable defelction even in the currently highest attainable fields. We show that the magnetic moment of a particle containing only a few atoms can be unambiguously determined when results from photo-detachment spectroscopy experiment which when combined with high level theoretical calculations is shown to be able to accurately determine the magnetic moments of small clusters.

Support from Grant N00014-02-1-4079 ONRIFO to atttend the conference is aknowleged. This work is supported part by a grant from the Department of Energy Number DE FG02-96-ER45579, Conacyt 32276-E, We thank Dr. M. Bowers for suggssting calculatios of transitions from neutral to cataion clusters. We are also thankful to Dr. L.S. Wang for providing us with the photo-detachment spectra.

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Charge Distribution and EFGs in Cuprates using the LDA+U Method

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It is well known that conventional bandstructure calculations based on LSDA fail to predict the correct magnetic and/or insulating ground state of many late transition metal oxides. This is in particular true for the non-superconducting parents of the high Tc cuprates, which are antiferromagnetic (AF) insulators, whereas band theory predicts them as non-magnetic metals. Various schemes for improvements with more or less empirical character have been put forward and the LDA+U method is one of them. Of course, LDA+U calculations do get the proper ground state for these AF cuprates, but here we investigate whether LDA+U also leads to correct charge densities in these systems.

The electric field gradient (EFG) depends sensitively on the non-sphererical charge distribution around an atom. It can be measured very accurately and thus provides a sensitive test of the quality of a calculation. Previously we have found, that the EFGs in both, doped and undoped cuprates, is well described by conventional LDA calculations for all atomic sites except the Cu-site (Cu2) in the CuO_2 planes, that is crucial for superconductivity. For these Cu2-sites the theoretical Cu-EFG is too small by a factor of two.

Application of the LDA+U method gives a significant improvement of this situation, although the results depend (to some extend) on the value of U and the specific form of the LDA+U method. In general the anisotropy of the charge density around the planar Cu site is enlarged, the Cu d-hole gets solely $d_{x^2-y^2}$ character and the resulting EFG increases and agrees well with experiment. The EFGs at the other sites are almost uneffected and remain in good agreement with experiment too.

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Magnetism Under the Scanning Tunneling Microscope

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In the frontier field of nano-magnetism understanding complex magnetic structures is crucial. We show that the spin-polarized scanning tunneling microscopy (SP-STM) and spectroscopy (SP-STS) offers a great potential to unravel complex magnetic superstructures on different length scales. We extended the model of Tersoff and Hamann to the situation of an STM with a spin-polarized tip with an arbitrary magnetization direction and a sample with an arbritary magnetic structure and discuss the different operation modes of a SP-STM: We show that the spectroscopy mode is ideal to analyse complex magnetic structures on a mesoscopic length scale created by atomic-scale ferromagnetism and we propose the application of the constant current mode of a SP-STM to the investigation of surfaces of complex atomic-scale magnetic structures of otherwise chemically equivalent atoms. We gave evidence of these capabilities of the SP-STM in terms of the first unambigious proof of two-dimensional antiferromagnetism in magnetic monolayer films on non-magnetic substrates predicted already in 1988. We demonstrate the potential of this approach applying it to resolve more complex magnetic structures such as the magnetic structure for Cr/Ag(111), which we found on the basis of first-principles vector spin-density total-energy calculations to be a coplanar non-collinear periodic Néel state. At last it is shown that the nanoscale magnetic structures can be observed even with a non-magnetic tip, by exploiting (the static limit of the linear dichroism) the spin-orbit contribution in the ballistic cross-section of the STM.

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Micromagnetic Modeling at Finite Temperature

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The Landau-Lifshitz-Gilbert equation describes the time dependence of magnetization at each point in a material as precession around a local magnetic field. The local field has contributions from effects such as, e.g., exchange, magnetostatics, and crystalline anisotropy. Short length-scale processes occuring at high frequencies, i.e. thermal fluctuations, can be incorporated as a randomly fluctuating field at each point in space, whose magnetitude is related to the temperature by the fluctuation-dissipation theorem. This finite-temperature micromagnetic model was used to model nanoscale magnetic pillars with diameters on the order of 10 nm and lengths on the order of 100 nm. Numerical integration of the model indicates that magnetization reversal occurs via a spatially inhomogeneous mode that is different from the well-known curling mode.

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Electronic and Magnetic Structure of a Room Temperature Magnetic Semiconductor: Ilmenite-alpha-Hematite

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There has been much interest in doping traditional semiconductors such as GaAs, InAs, InSb, GaN and GaP with Mn or other transition metals in order to obtain room temperature magnetic semiconductors. Some of the goals of this research have been a Curie temperature exceeding 350K and the possibility of both n- and p- type doping. An alternative approach is to investigate non-traditional semiconducting materials that are known to be magnetic at room temperature. Examples of such material are solid solutions of the minerals ilmenite and alpha-hematite. These materials were extensively investigated in the 1950's because of the puzzle presented by alpha hematite which has a tiny moment (0.002 Bohr magnetons/Fe atom) and a large Curie temperature (1000K) and because of the problems that these minerals caused to the young field of paleomagnetism. Understanding of the electrical and transport properties of these materials was greatly hampered by the lack of fully dense samples. Recently we have been able to obtain both dense ceramic samples and epitaxial films. These materials appear to have truly remarkable properties (exceeding the goals mentioned above) that we are attempting to understand and exploit.

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Multi-Scale Modeling of Magnetic Materials

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The micromagnetic modeling of magnetic materials has been undeniably successful in developing an understanding of basic magnetisation reversal mechanisms in a variety of technically important materials. However, the formalism is based on a continuum approximation. Within this formalism the magnetostatic energy can be calculated exactly, however the fundamental exchange interaction can only be calculated within an approximation valid only for long wavelength magnetisation fluctuations. Many physically and technically important magnetic materials have a granular structure with a characteristic lengthscale of the order of tens of nm. It is increasingly clear that furture developments in micromagnetism will require the introduction of atomic lengthscale information into the micromagnetic approach. The current situation will be reviewed with consideration of the problem of magnetisation structures in quantum constrictions. Equally important is the problem of time scales. In the case of magnetic recording, information is written in characteristic times of around 1ns, whilst the stored information must bestable for years. The various formalisms for dealing with each characterstic timescale will be outlined and recent work on a time quantified Monte Carlo technique will be described.

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Non-Collinear Magnetism in Iron

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The properties of iron at high pressures have been studied using a non-empirical non-collinear tight-binding model. Good agreement for the bcc Tc at zero pressure is found. The face centered cubic (fcc) phase has an incommensurate magnetic structure, which leads to a huge thermal expansivity called the anti-Invar effect. The tight-binding model gives the correct non-collinear structure. No magnetism has been seen in experiments for hexagonal close-packed (hcp) iron, which is the stable high pressure form and is probably present in the Earth's core, but first-principles and tight-binding calculations show local magnetism is probable below 60 GPa. Including non-collinear magnetism greatly improves agreement with the equation of state for hcp-Fe. An effective Hamiltonian fit to the model energies will be presented, and finite temperature properties of the model from Monte Carlo simulations will be discussed.

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The Spin-Density Wave in Chromium: Ground State and Impurity Hyperfine Fields

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Chromium has an antiferromagnetic spin-density wave ground state: moments on neighbouring atoms are antiferromagnetically coupled, but the magnitude of the moment follows a sine-like modulation with an amplitude of 0.62 μ_B. The wave is not commensurate with the lattice, and has a period of slightly less than 21 lattice constants. In the past, several attempts have been made to find what the DFT-prediction for the ground state would be. Due to the large size of the unit cell that models the wave (42 atoms), only recently total energy calculations that take into account the total wave were performed. LDA and GGA results gave different results, and different computational methods gave contradicting ground states. In this contribution, we present high-precision LAPW results that umabiguously show that DFT-LDA/GGA predicts the wrong antiferromagnetic ground state, with a moment that is twice as large as in experiment [1]. Work-in-progress about the experimentally important magnetic hyperfinefields on Cd and Sn impurities in the spin-density wave Cr will be reported.

[1] S. Cottenier et al., J. Phys. Condens. Matter 14 (2002) 3275-3283

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Spin-Injection from Half-Metals

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Half-metals constitute a promising class of materials for the injection of spin-polarized charge carriers into, for example, semiconductors. Interface states in the bandgap (whether induced by the half-metal or the semiconductor) are detrimental for the performance. The occurrence of interface states will be discussed in relation to the origin of the half-metallicity, the structure and the composition of the interface. The relevance of these interface states for the performance at finite temperature will be indicated.

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An Approach to Multiscale Simulations of Nonlinear Magnetization Dynamics

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Multiscale phenomena which include several processes occuring simultaneously at different length scales, and exchanging energy with each other, are widespread in magnetism. A mention can be made of nucleation of magnetization reversal at an atomic-scale defect or grain boundary, a domain wall breaking through a defect or the impact of the surface roughness on the domain wall dynamics.

We demonstrate that in such multiscale processes, a role of short-wavelength excitations dynamically generated near the defects is important, so that standard micromagnetic theory is not always sufficient for description of these phenomena. We present a novel coarse-graining approach to length scales coupling in dynamical magnetic modeling, which allows accurate treatment of microscopic defects in nanomagnets. The results of simulations performed on simplified model systems, where an atomic-scale variation of anisotropy and exchange represent defects in real systems, show that the coarse-graining approach achieves practically the precision of exact atomic simulations, while describing the system with a much smaller number of degrees of freedom.

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Influence of Spin-Orbit Coupling on the Electron Spectroscopy of Non-Magnetic Metals

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The Fano-effect denotes the observation that one can get a spin-polarized photo-current from non-magnetic materials due to the presence of spin-orbit coupling. A theoretical description of this effect in the valence band XPS of transition metals systems is presented that is based on the relativistic KKR band structure method. Corresponding results are found to be in very satisfying agreement with experiment. Recently, this type of experiment has been extended to ferromagnets. Using circularly polarized radiation a spin polarization could be found for a quantization axis perpendicular to the magnetization. Again a detailed and quantitative description could be given on the basis of the afore mentioned approach.

The Fano-effect has been used in the past to give a plausible explanation for the magnetic circular dichroism in X-ray absorption (MCXD) in spontaneously magnetized materials. It is shown that an external field may induce MCXD also in non-magnetic materials. A theoretical description of such an experiment is presented that is based on a combination of a fully relativistic linear response formalism and a corresponding treatment of the MCXD. In particular it is shown that application of the magnetic sum rules on corresponding spectra gives access to the spin and orbital element projected susceptibility of the system under investigation. This will be demonstrated for transition metal alloys.

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Magnetic Properties of Iron Nanowires on Copper

M. Eisenbach, B. Ujfalussy, G. Brown, G.M. Stocks
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We investigate the magnetic properties of iron chains in fcc copper using first principles calculations. Of main interest are linear chains of atoms aligned along different directions in this Cu matrix. The method of calculation we employ is the locally selfconsistent multiple scattering (LSMS) real space method for solving the LDA Kohn-Sham equation, which we have extended to perform fully relativistic calculations. This enables us to investigate the spin orbit coupling effects leading to magnetic anisotropies. With this approach we find that depending on the orientation of the atoms along the 100 or 110 direction in copper the ground state orientation of the magnetic moments in the chain is either ferromagnetic or anti-ferromagnetic. Furthermore we have investigated a classical model to describe the inhomogeneous distribution of iron in experimentally accessible systems, that might explain the reduced total magnetization observed experimentally.

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Self-Compensation in Manganese-Doped Ferromagnetic Semiconductors (*)

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We present theoretical evidence that the observed hole compensation in manganese-doped ferromagnetic semiconductors is due to interstitial manganese. We show that under the non-equilibrium conditions used during growth, interstitial Mn is readily formed near the surface by a simple low-energy adsorption pathway. In GaAs, isolated interstitial Mn impurities are electron donors, each compensating two substitutional Mn acceptors under p-type conditions. We show that partial compensation is a prerequisite for ferromagnetic order below the metal-insulator transition, and that the Curie temperature is highest when 1/6 of the Mn is interstitial.

(*) In collaboration with Andre G. Petukhov

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Versions of LSDA+U for Magnetic Structures

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A survey is given on the various possible L(S)DA+U versions if one does not restrict himself to a local orthonormal basis like LMTO for the Kohn-Sham functions. The cross features of the versions are compared for half-filled and nearly filled atomic shells. Results of full calculations for undoped cuprates and the problem of magnetic couplings in c-direction are discussed.

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Ferromagnetism and Spin-Orbital Compensation in Sm Intermetallics

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The electronic structure and magnetic properties of the ferromagnetic Sm intermetallics, $SmAl_2$ and $SmZn$, have been calculated within the LDA+U method. In contrast to LDA, which predicts a strong peak of 4f character in the density of states on the Fermi level, the LDA+U method predicts occupied 4f states well below the Fermi energy and empty ones well above this energy. We find a sizeable orbital magnetic moment, comparable in magnitude with the opposite oriented spin moment. This result is consistent with the recent observation of ferromagnetic spin ordering at the zero magnetization state.

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Exploring dynamical magnetism with Time Dependent Density Functional Theory (TDFT): From Spin Fluctuations to Gilbert Damping

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Using TDFT we study magnetic fluctuations in metals. Firstly, we investigate the failure of the adiabatic Local-Spin-Density-Approximation(ALSDA) to describe spin waves below the Curie temperature T_c and local moment fluctuations above T_c. Next we construct a gradient-dependent density functional which does not suffer from this problem. Finally, we show how our approach leads to a microscopic description of Gilbert damping.

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Magnetic Surface States in Two-Dimensional Transition-Metal-Based Compounds

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The electronic structure and the Fermi surface of the c(2x2) MCu/Cu(001) surface compound, M= Mn, Co, Ni, Fe, are studied on the basis of a layer multiple-scattering method as a function of magnetic ordering, surface buckling, and the results are used for interpretation of the experimental data. Analysis has been done in terms of the angle-resolved Photoemission yielding the Fermi surface, using its high surface sensitivity and virtue for energy and momentum resolution. Contrasting to Cu(001), two new features in MnCu surface compound forming hole-like Fermi surfaces are observed. One appears in the band gap close to the L-point of Cu(001) and is interpreted as a majority spin part of the spin-split Schockley surface state, the other one represents a minority Tamm-like spin state located at the manganese sites as concluded from the surface-resolved density of states. It is shown how the magnetic ordering within just half a monolayer of transition metal can essentially change the electronic structure of the surface provided the high quality and stability of the surface compound. It could also be conjectured that from all the transition metals, only Mn builds a stable two-dimensional magnetic compound, the others are either magnetically disordered or spin-restricted.

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Implementing Universal Quantum Computation with the Exchange Interaction

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A practical implementation of quantum computation using single-electron quantum dots is described. The quantum information is encoded in the electron spin. The electrons interact through the kinetic exchange interaction, and manipulation of this interaction alone (e.g. by varying gate voltages) allows any quantum circuit to be performed. Single electron manipulations via local magnetic fields, which are generally much more difficult to implement, are not required.

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Many - Body Effects at Transition Metal Surfaces: an Orbital Kondo Resonance in Chromium

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Electronic structure of Cr(001) surface is studied basing on the results of low-temperature STM investigations, first-principle electronic structure calculations, and many-body model considerations. A surprisingly narrow peak near the Fermi level found by the scanning tunneling spectroscopy is described as an orbital Kondo resonance near due to degeneracy of d_{xz}, d_{yz} surface states. This picture gives a naturalexplanation for a real-space STM image near imperfections as well as for the effect of atomic steps on the characteristics of the resonance. Friedel oscillations on the surface observed experimentally are described by ab initio calculations of the nonlocal susceptibility. It is shown that sp parts of the Fermi surface give main contibutions to the Friedel oscillations.

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Phase Diagram of the Symmetric and Asymmetric One-dimensional Periodic Anderson Models

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We have studied the ground-state properties of the symmetric and asymmetric one-dimensional periodic Anderson model as a function of band filling and the model parameters (V, U and E_F) using the local mean-field (LMF) approach. We have constructed the phase diagram for both cases and have calculated the energy, local moment, and occupation number of the f-level. The LMF approach can reveal the basic properties of the system throughout the entire parameter space. For the symmetric case (E_F=-U/2), close to quarter- and half- filling the antiferromagnetic phase is the ground state. For intermediate band-filling there is a continuous second-order phase transition to a ferromagnetic state. At quarter filling there is a transition from a metallic paramagnetic state to an insulating antiferromagnetic state as the on-site Coulomb interaction increases. The asymmetric case is treated in the mixed-valence regime ($E_F = 0$). At half-filling the ground state is antiferromagnetic while at or close to quarter filling it is paramagnetic. Below half-filling the ground state becomes ferromagnetic, suggesting that doping destroys rapidly the antiferromagnetic f-f spin correlations. For small values of U we find a paramagnetic state at all band fillings. Results for the average occupation number of the f-level compare well with density matrix renormalization group calculations.

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Correlation Effects in Magnetic Properties:
A First Principles Dynamical Mean Field Approach

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We will outline current efforts to obtain a first principles approach to the calculation of the properties of solids which is particularly suitable to treat magnetic systems. It is accurate both in the atomic limit as well as the band limit, and can be used to compute total energies as well as one particle spectra and transport properties.

The essential physical input is an improved treatement of the local correlations. In many cases this has already resulted in significant improvements over the results of the density functional approach. We will illustrate this point using as an example the archetypical itinerant ferromagnets iron and nickel. An improved treatement of the local correlations allows a more accurate description of the finite temperature susceptibility, the photoemission spectra and the low temperature magnetic anistropy of these systems.

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Wannier State Analysis of Insulating Ferromagnetism in $La_4Ba_2Cu_2O_{10}$

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The exceptional insulating ferromagnetism, discovered in the brown phase of half-filled $La_4Ba_2Cu_2O_{10}$ (La422), poses a great challenge in our quantitative theoretical understanding of quantum magnetism. It is even more puzzling with the recent discovery of the "normal" antiferromagnetism of the isostructural $Nd_4Ba_2Cu_2O_{10}$ (Nd422). With a newly developed scheme, in which the reformulated ab initio 2nd quantized Hamiltonian is represented based on energy-resolved all-electron Wannier states (WSs), the origin of the ferromagnetism is identified to be the intersite direct exchange between WSs. The calculated parameters (t,U, and J) indicate that this mechanism overwhelms the Hubbard-type superexchange considered in existing analysis. By contrast, Nd422 is shown to develop the experimentally observed antiferromagnetism via its characteristics of a 1D chain. Contrary to current assumption, in both compounds, the dominant in-plane coupling turns out to be not with the nearest neighbors, but with the ones above/below them. These results agree very well with many aspects of current experimental observations. The energy-resolved WSs are shown to be ideal for studying magnetism from first principles, and the spatial distribution of the WSs reflects that of the spin moment. The crucial role of the chemical replacement is analyzed with additional calculation on La422 under pressure, which not only reproduces observed magnetic order, but also suggests an intriguing pressure-induced ferromagnetic to antiferromagnetic transition upon higher pressure.

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Spin Dynamics Simulations of Excitations and Critical Dynamics in a Heisenberg Antiferromagnet

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Spin dynamics simulation methods have developed sufficiently that they now provide a powerful tool for the examination of excitations and dynamic critical behavior in magnetic models. From the Fourier transform of the space-displaced, time-displaced correlation functions the dynamics structure factor S(q,w) can be extracted. We shall describe modern decomposition methods for the time integration and present results for a classical, Heisenberg antiferromagent on a simple cubic lattice. This model is an excellent "testing ground" since it is expected to describe the magnetic behavior of $RbMnF_3$ quite well. We shall compare our results with theoretical predictions as well as with detailed neutron scattering data. *dlandau@hal.physast.uga.edu*

Non-Quasiparticle States in Half-Metallic Ferromagnets

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The Half-Metallic Ferromagnets are an important class of itinerant electron materials because of their potential for spin-electronics. The Heusler alloy NiMnSb was the first material predicted to be a Half-Metallic Ferromagnet (HFM) in the framework of the Local Density Approximation (LDA) with the Fermi level in the gap for one of the spin directions. We study the effects of strong correlation between spin and charge degrees of freedom in NiMnSb within the Dynamical Mean Field Theory (DMFT). Based on LDA+DMFT electronic structure calculations we present the first evidence for the existence of non-quasiparticle states lying in the gap of the minority spin channel just above the Fermi level.

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The effect of the exchange splitting on the magnetic anisotropy of Ni

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The Slater-Koster tight-binding method has become an important computational tool for band structure calculations. The method is accurate and computationally very fast compared to first-principles calculation. For this reason we have extended this method to include spin-orbit coupling, a property that is needed in the magnetic anisotropy calculation for Fe, Ni and Co. Using the three-center orthogonal parameters of Ref.[1], Schneider and Jansen [2] have calculated the magnetic anisotropy energy (MAE) for the ferromagnetic materials such Fe, Co and Ni, and found the value for Ni is in disagreement with the experimental value. It has been suggested that this discrepancy comes from strong correlation effects or from the wrong Fermi surface topology. To check this results we have performed MAE calculations using the TB parameters [3] adjusted to reproduce the experimental Fermi surface topology and exchange splitting, however we did not find a substantial improvement in terms of the agreement with the experiment. We conclude that the conjecture that the MAE in Ni is adversly affected by incorrect Fermiology and/or exchange splitting is probably incorrect.

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Spin-Polarised Transport in Hybrid Ferromagnetic-Superconducting Nanostructures

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Recent results for spin-polarised transport in hybrid ferromagnetic-superconducting nasnostructures will be presented. It is known that for a diffusive magnetic multiplayer, the conventional giant magnetoresistance (GMR) ratio drops to zero when one of the normal contact become superconducting. Instead, the magneto resistance exhibits an extremum when magnetic moments of adjacent F-layers are approximately at right angles. In the presence of spin mixing, either through spin-orbit coupling or non-collinear magnetic moments, I show that conventional GMR is restored.

When two ferromagnetic wires are in contact with a superconductor, it is known that novel non-local effects can occur, due to the blocking of Andreev reflection in the half-metallic limit. A survey of different transport regimes is presented.

Finally results are presented for spin-dependent electronic transport across ferromagnet / superconductor ballistic junctions modeled using tight-binding Hamiltonians with s, p and d orbitals and material-specific parameters. By accurately modeling the band structure of the bulk materials, one can reproduce the measured differential conductance of Cu/Pb nanocontacts.In general however, the spin polarization P of the current is completely different from the bulk polarization P. Eg for Co we find a bulk polarization of -0.4, whereas for the Co/Cu interface P=+0.4 and for the Co/Ir interface P=-0.01.

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Magnetic Properties of Transition Metal Impurities in SiC

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Local spin density functional calculations were carried out for the entire series of $3d$ transition metal impurities in 3C-SiC using the linear muffin-tin orbital method and 64 atom supercells. Si site substitution, preferred from the point of view of formation energies, gives low spin states with the spin-splitting being dominated by the crystal field $e - t_2$ splitting. For example, for Mn, Cr a magnetic moment of 1,2 μ_B is found. The C site substitution gives high spin states for the early transition metals but is not preferred energetically. The magnetic moments are well described in terms of a simple defect level filling scheme. When neighboring TM pairs are considered, the magnetism is generally quenched except for Mn and Cr on the Si site. Mn however gives an antiferromagnetic alignment while Cr gives a ferromagnetic alignment. This is surprising from the point of view of the Anderson-Hasegawa model. A tentative explanation is offered.

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Large Magnetic properties of YCo_5 and $SmCo_5$

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We have studied the magnetic moments and magnetic anisotropy energy (MAE) of YCo_5 and $SmCo_5$ using full-potential LAPW electronic structure calculations. Most previous calculations of the MAE for YCo_5, using LDA for the exchange-correlation potential, have found values significantly smaller (∼0.6 meV/f.u.) than experiment (∼3.8 meV/f.u.). The rest of the MAE is attributed to orbital polarization (OP) effects. Our full-potential LAPW calculations using GGA instead of LDA and including spherical corrections give values ∼1.5 meV/f.u. and improves to ∼3.5 meV/f.u. when LDA+U(SIC) corrections were included for the Co d levels. The Co magnetic moment, unlike the prediction of the virtual crystal approximation, of $YCo_{5-x}Cu_x$ and $Y_2Co_{7-x}Ni_x$ decrease slowly with impurity concentration until dropping suddenly to zero at a critical dopant concentration. Significant improvement is found for the MAE in $SmCo_5$. GGA calculations give MAE for $SmCo_5$ of ∼-11 meV/f.u. which improves when including LDA+U(SIC) to ∼11 meV/f.u., in good agreement with the experimental value lying between 12 and 16 meV/f.u.

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Optimized Antiferromagnetic Orthophosphates for Lithium Battery Cathodes.

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The effects of spin-polarization and magnetic ordering on the amplitude of the intercalation voltage of LiXPO4 (X=Mn, Fe, Co) oxydes is investigated. We demonstrate that the antiferromagnetism, both observed experimentally and by our ab-initio calculations, allows a larger hybridization of the bands of the transition metal ion with a wide and fixed band formed by the Li-P-O states, generating a gain of energy with respect to the non-magnetic calculation. The same kind of behavior was obtained for MnPO4 and FePO4, with this time a larger hybridization between Mn or Fe with the P-O band in the case of the antiferromagnetic calculation. However, the position of the metallic peaks of Co and Ni close or inside the P-O band of the CoPO4 and NiPO4 compounds raises no major differences between their antiferromagnetic and non-magnetic electronic structure, bringing no additional stabilization energy to the magnetic configuration. This asymmetrical energetical behavior between LiCoPO4 and CoPO4, or LiNiPO4 and NiPO4, explains the sudden enhancement of the Li intercalation voltage for both these candidate-batteries.

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Ab-Initio Calculation of the Magnetic Anisotropy Energy of Fe-V Multilayers

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The magnetic anisotropy energy (MAE) of the Fe_2V_6, Fe_3V_5 and Fe_4V_4 multilayers are investigated using first principles spin–polarized and relativistic band structure calculations based upon the full–potential linearized muffin–tin orbitals (FP–LMTO) method. A strong difference in the MAE and the easy axis of magnetization (calculated for the experimental lattice parameters) is observed between the three studied tetragonal distorted multilayer systems, with an easy axis of (001), (110) and (100) for Fe_2V_6, Fe_3V_5 and Fe_4V_4, respectively. The MAE of the Fe_2V_6 and Fe_4V_4 multilayers agree well with the experimental data. The origin of this difference of behavior is analyzed, *via* a study of the influence of the atomic volume as well as a relaxation study of the multilayers with respect to the tetragonal deformation. The important role played by the c/a axial ratio, imposed by the alloying effects, are outlined. The magnetic anisotropy coefficients entering the expression of the MAE, as a function of the directional cosines, are extracted from a series of calculations for four independent spin directions. Finally, the band filling effects on the MAE have been analyzed as well as the different contributions of the reciprocal space.

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Magnetic Inclusion Compounds: The Alkali-Electro Sodalites and the Rare-Earth Containing Clathrates

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The use of porous framework structure gives several interesting new possibilities for magnetic materials. We will present the alkali-electro-sodalites where the framework stabilizes otherwise unstable magnetic nano-cluster and the rare earth filled clathrates where the magnetic dopants modify the electronic structure and transport properties of the framework. We use the APW+lo method together with the lda+U method, as embodied in the WIEN2k code, to study these compounds.

Sodalites are the simplest of the zeolite structures and can be described as a bcc arrangement of β-cages built from corner-shared SiO_4 and AlO_4 tetrahedra. The negative charge of the (AlO_2^-) unit can be compensated by three alkali cations (A^+) inside each cage. If each sodalite cage is doped with an extra alkali ion the extra electrons form a regular array of F-centers at the center of each cage. The sodium and potassium electro sodalites have been found to show anti-ferromagnetic order at low temperature and the magnetism is due to the formation of a narrow s-like band in the sodalite band-gap.

We have studied these compounds under pressure. In agreement with experiment we find that the spin-polarized F-center bands in SES initially narrow with applied pressure and consequently a high critical pressure for the magnetic insulator to nonmagnetic metal phase transition is predicted (127 GPa). Surprisingly the critical pressures of the potassium and rubidium doped sodalites are found to be an order of magnitude lower (20 GPa and 13 GPa respectively). The collapse of magnetism is found to occur when the unoccupied p-states of the alkali atoms mix with the sodalite bands.

The clathrates are semi-conductors with large cages. The europium containing clathrates have been found to exhibit both ferro magnetic and anti-ferromagneticorder. We show that the magnetic order depends on the doping level, in that the valence bands have an anti-ferromagnetic coupling and the conduction bands a ferro magnetic. This means that the carrier mobility is strongly dependent on the doping sign and concentration.

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Ferromagnetism in Dilute Magnetic Semiconductors

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Current interest in achievement of ferromagnetism at ambient temperatures has led to the investigation of the mechanism that stabilizes ferromagnetism in transition metal doped semiconductors. We report on three types of studies:

(1) GGA calculations on total energies, acceptor levels and electronic structure of V, Cr, Mn, Fe, Co and Ni in GaAs, GaN and GaP [1]: By varying the transition metal impurity as well as the semiconducting host independently [1], we have constructed models with realistic interaction strengths to derive certain basic principles to understand ferromagnetism in these systems. We find a conventional double-exchange like mechanism at work in the case of systems like GaN:Mn which have dominantly Mn d character at the Fermi level. On the other hand, in systems such as GaAs:Mn which have dominantly As p character at the Fermi level, the mechanism is novel and is similar to what was proposed earlier for Sr2FeMoO6 [2].

(2) GGA calculations on substitutional + interstitial Mn complexes in GaAs [3]: We find the formation energy for Mn at an interstitial site is comparable to the energy required to substitute a Ga site with Mn under certain experimental conditions [3]. Charge neutral complexes between substitutional Mn and interstitial Mn are found to be strongly stabilized by Coulomb interactions. These complexes exhibit charge compensation, but surprisingly favor a ferromagnetic coupling between the substitutional Mn atoms.

(3) Calculations of Mn in chalcopyrites: In recent times, Mn doped CdGeP2 has been found to exhibit room temperature ferromagnetism [4]. In Ref. [5] we have considered the interaction of intrinsic defects with substitutional Mn on Cd and Ge sites to elucidate under what experimental ferromagnetism can be achieved.

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Instability of bcc Ferromagnetic Fe Under Pressure

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Under pressure elastic constants generally increase as atoms overlap and strong repulsive forces develop. However magnetic moments decrease under pressure and reduce the elastic constands of magnetic materials as unbalanced spin distributions cost more kinetic energy. Ferromagnetic bcc Fe shows both these pressure effects. Elastic constants rise initially, but then fall as magnetic moments decrease. The shear constant C' of bcc Fe vanishes at 1500 kbar and bcc Fe becomes unstable. This behavior has been obtained with first principles calculations by a method which finds the structural and elastic properties of bcc Fe directly as a function of pressure p. The method defines at each P a Gibbs free energy whose minimum as a function of structure gives the equilibrium state at P. Elastic constants are then calculated from second strain derivatives of the free energy at the equilibrium state, whereas it would be wrong to use the second strain derivatives of the energy. The free energy also shows that a body-centered tetragonal (bct) phase with $c/a = 0.88$ forms at 1300 kbar with C' negative, but that at 1825 kbar C' becomes positive and the bct phase is stable. This bct phase fits the observation of a phase of Fe at 2000 kbar and 2000°.

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Theory of Spin-Dependant Tunneling in Magnetic Multilayers

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Rigorous theory of the tunneling magnetoresistance (TMR) based on the real-space Kubo formula and fully realistic tight-binding bands fitted to an ab initio band structure is decribed. It is first applied to calculate the TMR of two Co electrodes separated by a vacuum gap. The calculated TMR ratio reaches some 65% in the tunneling regime but can be as high as 280% in the metallic regime when the vacuum gap is of the order of the Co interatomic distance (abrupt domain wall). It is also shown that the spin polarization P of the tunneling current is negative in the metallic regime but becomes positive P $\sim$ 35% in the tunneling regime. Calculation of the tunneling magnetoresistance of an epitaxial Fe/MgO/Fe(001) junction is also described. The calculated optimistic TMR ratio is in excess of 1000% for an MgO barrier with 20 atomic planes of MgO and the spin polarization of the tunneling current is positive for all MgO thicknesses. Finally, it is demonstrated that the TMR ratio calculated from the Kubo formula remains nonzero when one of the Co electrodes is covered with a copper layer. It is shown that nonzero TMR is due to quantum well states in the Cu layer which do not participate in transport. Since these only occur in the down-spin channel, their loss from transport creates a spin asymmetry of electrons tunneling from a Cu interlayer, i.e. nonzero TMR. Numerical modelling and coherent potential approximation are used to show that diffuse scattering from a random distribution of impurities in the barrier may cause quantum well states to evolve into propagating states, in which case the average TMR tends to zero but large quantum oscillations of TMR about zero average remain. The origin of such quantum oscillations is discussed and the theoretical predictions for a junction with a nonmagnetic interlayer are comparedwith recent experimental results for a tunneling junction with an allumina barrier and an epitaxial copper interlayer.

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Correlated metals and the LDA+U method

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The purpose of this work is to investigate existing recipes for LDA+U calculations from the point of view of (i) their "first-principles"justification, (ii) their practical usefulness, and (iii) their effect on magnetic properties. Since in case of strongly correlated systems the LDA+U ideology is at least practically established, we shall concentrate more on the relatively new area of applying LDA+U to moderately-correlated, metallic systems. We explicitely calculate Stoner paramters for two available LDA+U functionals and show that neither of them correctly describes the essential physics of the correlated metals (e.g. FeAl) : (i) reducing the band dispersion by dressing of the one-particle excitation, and (ii) spin fluctuations near the quantum critical point.

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A Model of Magnetization Thermal Fluctuations in Mono-Domain FePt Particles

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The temperature dependence of magnetic properties of mono-domain FePt particles has been studied using model for the energetic of magnetization thermal fluctuations based on the effective Hamiltonian constructed on the basis of first-principles calculations of non-collinear configurations. We use combination of infinitesimal and finite angle rotation approaches to map in the realistic manner energies of thermal fluctuation to the relatively simple effective Hamiltonian. On the basis of these calculations we propose statistical model of the thermal fluctuations in fct ordered FePt mono-domain particles. In considered case of the ordered alloy containing magnetic (Fe) and non-magnetic element (Pt), we find that induced atomic magnetic moment of Pt produces main distinct feature of energetic of the thermal fluctuations. This feature has been treated within a model effective Hamiltonian analyzed using mean-field approximation and numerically within the Monte-Carlo method. Results indicate importance of the exchange interaction anisotropy distribution on temperature dependence of magnetic properties. The effects of finite size and surface atoms is also discussed in the context of explanation of observation for the critical temperature of nano-composite FePt:Bi_2O_3 films

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Spin-Filter Effect in Metallic Nanowires

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We present ab-initio calculations for metallic nanowires with a diameter of few atoms. The electronic structure is calculated using the screened Korringa Kohn Rostoker (KKR) Green's function method, while transport properties are obtained by means of the Landauer formalism. We focus on the effect of scattering due to transition metal impurities on the conductance of a Cu wire. For a single impurity atom, our results show a reduction of the transmission for energies at the impurity d state. For a defect pair, however, quantum interference effects lead to a complicated energy dependence of the conductance.

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Slow Jahn-Teller Dynamics And Carrier Transport In Diamagnetically Diluted Perovskite Manganites

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To get information on the interplay of magnetic and lattice systems in manganese perovskites, electric carrier transport and nuclear spin-lattice relaxation have been studied in diamagnetically diluted manganite single crystals of LaGa1-xMnxO3, with the concentration of Mn ions, x, varied from 0 to 100%. The electric conductivity is found to be determined by a small polaron hopping model with an activation energy of 120 $\sim$ V 720 meV depending on Mn concentration. Nuclear spin-lattice relaxation of 71Ga in the samples with low concentration of Mn ions increases upon heating in the range of temperatures studied (190K-380K). In this case, the relaxation mechanism is governed by quadrupolar interactions, as proved by relaxation kinetics at various resonance transitions and by comparison of the relaxation rates for the 71Ga and 69Ga isotopes. In the crystals with higher Mn concentration (2%-20%), the magnetic mechanism of nuclear relaxation became dominant. In the 2% compound, temperature dependence of the relaxation rate demonstrated maximum at 290 K, allowing direct determination of the correlation time, $\sim$ 2*10-9 sec. At x¿2%, the nuclear relaxation rate decreases steeply as temperature increases. The experimental data point to the magnetic mechanism of relaxation through thermoactivated fluctuations, with the value of the activation energy $\sim$ 50 meV, same for all the crystals studied. This value is consistent with the critical temperature of the cooperative Jahn-Teller phase transition into the O-phase typical of CMR manganites. In our opinion, these results can be explained by the presence of quasi-static Jahn-Teller distortions (polarons) associated with Mn 3+ ions in the LaGaMnO3 crystals.

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In-Plane Uniaxial Anisotropy at the Fe/ZnSe(001) Interface

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We present a detailed study of the in-plane magnetocrystalline anisotropy (MCA) and its connection to the electronic bonding at an interface between a cubic ferromagnet and a cubic semiconductor, Fe/ZnSe(001). In particular, a uniaxial MCA is found. This is maybe surprising since the calculations are for perfect interfaces, but the effect is traced down to the sp^3-bonding between the semiconductor and the first monolayer of Fe. A uniaxial in-plane MCA is consistent with what is observed in general for bcc Fe/semiconductor interfaces, which jas been a puzzle since its first observation. We will discuss our results in connection with existing models. It is also shown how this uniaxial symmetry is cancelled in a multilayer structures, leading to four-fold anisotropy. The calculations were performed using a full-potential linearized augmented planewave method (FP-APW+lo), which is a computationally more efficient version of the traditionally linearized metod, FLAPW. The spin-orbit induced MCA was studied through the force theorem, as well as through fully relativistic self-consistent calculations. The magnetic anisotropy is presented for several different Fe/ZnSe(001) systems, with three or five monolayers of Fe grown on a five atoms thick representation of the semiconductor, and with Zn terminated as well as Se terminated semiconductor interfaces.

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Tight-binding v. LDA+U in FeAl

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Recently[1], we calculated the Stoner criterion $N(E_f)I$ for ferromagnetism in FeAl. We found that $N(E_f)I=1.06$ at the experimental value of the lattice parameter while it is below 1 at the LDA lattice constant. Other workers[2] have determined a magnetic moment of 0.7mB again at the experimental value of "a". Since experimentally B2-FeAl is believed to be non-magnetic there is great interest in resolving this issue. A new theoretical study[3] applying the so-called LDA+U approach argues that there is a range of U values that causes a lowering of the Fe-t2g states and a reduction of $N(E_f)$ sufficient to have $N(E_f)I¡1$. We want to advocate that as long as the value of U is treated in the LDA theory as an adjustable parameter there is nothing to be gained by using the complex LDA+U formalism. An accurate 3-center-orthogonal tight-binding Hamiltonian that reproduces very well the LDA band structure leads to exactly the same result as the LDA+U theory by varying the value of the t2g Fe on-site parameter which plays the role of U.

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2nd and 4th-order Anisotropies in Molecular Magnets

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Recently a class of transition-metal containing molecules have attracted significant experimental interest because they retain their magnetic orientation at relatively high temperatures and because they exhibit quantum tunneling of magnetism. These molecular magnets, consist of approximately 70-200 atoms and are typically composed of 4-15 transition metal atoms which are held in place by organic ligands and anions. The fundamental figure of merit which governs these phenomena is the magnetic anisotropy which arises due to the spin-orbit interaction and other couplings between spin and spatial degrees of freedom. Recent calculations, within an all-electron density functional framework on the $Mn_{12}O_{12}(RCOO)_{16}(H_2O)_4$ and $Fe_8O_2(OH)_{12}(C_6N_3H_{15})_6$ and $Co_4(C_5NH_4CH_2O)_4(CH_3OH)_4Cl_4$ molecular magnets will be discussed within the context of recent experiments. In particular we compare the measured spin-ordering and magnetic tunneling fields to those determined from the density-functional-based magnetic anisotropy hamiltonian. We also will compare the calculated infrared and Raman spectra to recent experiments and discus how the vibrational properties influence the magnetic properties. Results are in good to excellent agreement with experiments depending on the system.

A brief review of the computational method, NRLMOL, which is a gaussian-orbital based all-electron density-functional method will be included in the talk. Various parts of this work were performed in collaboration with Drs. Jens Kortus, Shiv Khanna, Tunna Baruah and Noam Bernstein.

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Resonant Enhancement of Tunneling Magnetoresistance in Double-Barrier Magnetic Heterostructures

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We show that spin-dependent resonant tunneling can dramatically enhance tunneling magnetoresistance. Instead of conventional one-barrier magnetic tunnel junctions we consider double-barrier structures comprised of a semiconductor quantum well sandwiched between two insulating barriers and two ferromagnetic electrodes. By tuning the width of the quantum well the lowest resonant level can be moved into the energy interval where the density of states for minority spins is zero. This situation leads to a great enhancement of magnetoresistance, which exhibits a strong maximum as a function of the quantum well width. The magnitude of this maximum depends exponentially on the width of the barriers and exceeds several thousand percent for generic one-band model. As a practically important example, we considered multiband resonant tunneling of holes in GaMnAs/AlAs/GaAs/AlAs/GaMnAs double-barrier heterostructures. We demonstrate that even in the presense of the spin-flip processes magnetoresistance exceeding 800% is achievable in these junctions.

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Spin-Spin Interactions and Ferromagnetism in Mn-Doped GaAs

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Ferromagnetism in Mn-doped GaAs is generally believed to be mediated by holes arising from substitutional Mn. Measured hole concentrations are much smaller than expected from simple electron counting, for unknown reasons. We present theoretical evidence that the observed hole compensation in manganese-doped ferromagnetic semiconductors is due to interstitial manganese. In GaAs, isolated interstitial Mn impurities are electron donors, each compensating two substitutional Mn acceptors under p-type conditions. We demosntrate that below metal-insulator phase transition ferromagntic interactions occur only between Mn acceptors in different charge states. We develop a two-color percolation theory of ferromagnetism in GaMnAs and show that partial compensation is a prerequisite for ferromagnetic order below the metal-insulator transition, and that the Curie temperature is highest when 1/6 of the Mn is interstitial. We compare our model with existing models of ferromagnetism in GaMnAs.

Magnetic Properties of Mn-N Compounds

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An electronic structure study is presented of MnN compounds. MnN has a slightly distorted rocksalt structure and if antiferromagnetic with the AFM-I (001) $n = 1$ ordering. Mn_3N_2 forms an ordered vacancy compound of rocksalt with N vacancies every 3 (001) layers with a AF (001) $n = 1$ ordering Full-potential linear muffin-tin orbital calculations were performed for MnN in the nonmagnetic, ferromagnetic, AFM-I and AFM-II (i.e. (111) $n = 1$) forms. The results indicate that the AFM-I state is below the FM state while the AFM-II state is above the FM state. This indicates exchange couplings $J_1 < 0$ and $J_2 > 0$ with $|J_2| > |J_1|$. This can be understood in terms of the double exchange mechanism via the intervening N. If we map this model on the classical Heisenberg Hamiltonian, we find that with such interactions, the model is frustrated. The stabilization of the AFM-I ordering is presumably related to the slight c/a reduction. In Mn_3N_2, we find a larger energy difference between AF and FM states with still the AF ordering having lower energy. Other spin configurations are under study to extract the exchange interactions. Results on the elecronic densities of states provide insights in the origin of the magnetic moments. This indicates exchange couplings $J_1 < 0$ and $J_2 > 0$ with $|J_2| > |J_1|$. This can be understood in terms of the double exchange mechanism via the intervening N. If we map this model on the classical Heisenberg Hamiltonian, we find that with such interactions, the model is frustrated. The stabilization of the AFM-I ordering is presumably related to the slight c/a reduction. In Mn_3N_2, we find a larger energy difference between AF and FM states with still the AF ordering having lower energy. Other spin configurations are under study to extract the exchange interactions. Results on the elecronic densities of states provide insights in the origin of the magnetic moments.

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New Magnetic Semiconductors $CuCr_{1.5}Sb_{0.5}S_4$ with $CoCr_2S_4$

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A giant negative (for the compound with x=0.25 - 16% in a magnetic field of 27 kOe, with x=0.5 - 24% in a field of 30 kOe) has been found in the new magnetic semiconductors $x CoCr_2S_4$-(1-x)$CuCr_{1.5}Sb_{0.5}S_4$, (x=0.25;0.5). Magnetoresistance in practically absent in $CuCr_{1.5}Sb_{0.5}S_4$ and does not exceed 2% in $CoCr_2S_4$. The giant magnetoresistance and the positive value of paramagnetic temperature Kuri are evidence for the exictence of afmons in compounds with Co. The sample which was reaserched can use in technics of sensors of magnetic field.

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Parameter-Free Calculation of the Exchange Interactions in Complex Magnetic Systems

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The frozen-magnon approach to the calculation of the exchange interactions in complex magnetic crystals with many-atomic unit cells is discussed. The scheme is applied to the study of the spin-wave spectrum, interatomic exchange parameters and Curie temperature in diluted magnetic semiconductors (DMS) of the III-V type. The main attention is given to the study of the role of charge carriers in the formation of the long-range ferromagnetic structure with relatively high Curie temperature already for low concentrations of the 3d impurity. Also an attempt to understand unusual magnetic properties of Laves phase compounds YFe_2 and UFe_2 within a simple frozen-magnon calculational scheme is briefly outlined.

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Linear Response Calculations of Lattice Dynamics in Antiferromagnetic Insulators

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We introduce a new linear response method to study lattice dynamical properties of materials with strong correlations. It is based on a combination of dynamical mean field theory of strongly correlated electrons and local density functional theory of electronic structure of solids. Using static limit we illustrate the applicability of the method on phonon dispersions of a prototype Mott insulator NiO. Our results generally show a much better agreement with experiment as compared to the local density predictions.

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On the Microscopic Origin of Exchange Bias: The Role of Anisotropic Exchange

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Despite resent progress in understanding numerous theoretical aspects of exchange bias systems, the microscopic origin of the exchange bias effect is still mostly unclear. One central issue is the apparent contradiction between the random field model and the spin flop coupling mechanism. In the former the unidirectional coupling across the antiferromagnet-ferromagnet (AFM-FM) interface is ascribed to a net interfacial moment along the AFM easy axis, while in the latter the coupling is uniaxial and perpendicular to the AFM easy axis. For any reasonably sized AFM domain or grain the net coupling should be perpendicular to the AFM easy axis and exchange bias should vanish. Yet, in systems such as CoO/Fe_3O_4 perpendicular coupling is observed concurrently with exchange bias. We will show how this discrepancy can be resolved when anisotropic exchange at the interface is taken into account, which, unlike most bulk cases, does not vanish on grounds of symmetry. In particular we will show that within a random field approach, the Dzyaloshinsky-Moriya term yields unidirectional coupling of the correct order of magnitude. Furthermore, we will give examples of (and derive criteria for) epitaxial AFM-FM bilayer structures that show unidirectional coupling for fully compensated AFM interfaces.

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Atomic Structure, Binding Energy, and Magnetic Properties of Iron Atoms Supported on Polyaromatic Hydrocarbons

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The atomic structure, energetics, and properties of gas-phase cluster complexes containing coronene (C24H12) molecule and up to two iron atoms are studied for the first time using density functional theory and generalized gradient approximation for exchange and correlation. The geometries of the neutral and cationic iron-coronene complexes are optimized without symmetry constraint and by examining the possibility that iron atoms could occupy various sites via individual or bridging interactions. In both neutral and cationic complexes a single Fe atom is found to preferentially occupy the on-top site above the outer ring, while two Fe atoms dimerize and bind to outer bridge sites. The binding energy of neutral Fe2-Coronene defined with respect to dissociation into coronene and Fe2 is larger than that of Fe-coronene while reverse is true for the corresponding cations. Although the ionization potentials of these complexes are not very sensitive to the number of adsorbed Fe atoms, they are significantly reduced from those of the Fe atom or the coronene molecule. The photo-decomposition of cationic (Fen-coronene)+ complexes proceeds through the ejection of either coronene+ or (Fe-coronene)+ cations while in the case of neutral Fe2-coronene, the ejection of Fe2 is energetically preferred. The coupling between the Fe atoms remains ferromagnetic although the magnetic moment/atom is reduced from the free-atom value. The results compare well with recent mass ion intensity and photo-fragmentation experiments.

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Magnetism and Electronic Structure in $ZnFe_2O_4$ and $MnFe_2O_4$

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Density functional calculations are used to study magnetic and electronic properties of the spinel ferrites, $ZnFe_2O_4$ and $MnFe_2O_4$. Correct magnetic orderings are obtained. $ZnFe_2O_4$ is predicted to be a small gap insulator in agreement with experiment. $MnFe_2O_4$ is found to be a low carrier density half-metal in the fully ordered state. However, strong effects on the electronic structure are found upon partial interchange of Fe and Mn atoms. This shows that the insulating character may likely be due to Anderson localization associated with the intersite Mn-Fe disorder.

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The Onset of Magnetic Order in Fe and Co Films On and Embedded in Non-Magnetic Substrates

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On the basis of a first-principles electronic structure theory of finite temperature metallic magnetism in layered materials, we investigate the onset of magnetic order in thin films of Fe and Co(1-8 layers) on and embedded in non-magnetic substrates, specifically bcc-Fe/W(100), fcc-Fe/Cu(100) and fcc-Co/Cu(100). The thermally induced spin-fluctuations are treated within a mean-field, disordered local moment (DLM) picture and give rise to layer-dependent 'local exchange splittings' in the electronic structure even in the paramagnetic phase. These features determine the magnetic intra- and interlayer interactions which are strongly influenced by the depth at which the films are embedded. In uncapped Fe/W(100) we find intralayer ferromagnetic correlations in all thicknesses of the iron film except in the layer nearest the W substrate, in agreement with experiment. The interlayer couplings are also ferromagnetic and short-ranged. There are also ferromagnetic intra- and interlayer couplings throughout the Co films in fcc-Co/Cu(100). In Fe/Cu(100) system the top two layers are coupled ferromagnetically and the rest antiferromagnetically. Cu-capping has a profound effect upon the magnetic coupling in both Fe/Cu(100) and Co/Cu(100) with Tc showing an oscillating behavior as a function of the cap layer thickness as found experimentally. In contrast there is no dramatic effect when Fe films are embedded in W(100).

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Evidence for Antiferromagnetic Correlations in HCP Iron

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While direct measurements (Mössbauer spectroscopy) do not show any magnetism in the high pressure polymorph of iron, hexagonally close packed (hcp), density functional theory predicts an antiferromagnetically (afm) ordered superstructure with wave-vector at the M-point on the Brillouin zone boundary (afmII) that is stable up to a pressure of approximately 50 GPa. This structure yields much improved agreement of experimental elastic data, including the equation of state and aggregate moduli compared to the non-magnetic case. We provide direct evidence of magnetic correlations in hcp iron by considering the influence of spin-phonon interactions for afmII on the zone center transverse optical TO phonon modes in hcp iron. We compute the frequencies of the Raman active TO modes with a frozen phonon approximation using the LAPW method. With afm correlations we can quantitatively explain the experimental measurements of two Raman active modes in hcp iron which is in contrast to the fundamental prediction of one doubly degenerate mode. Combined with the explanation of superconductivity in hcp iron by magnetic correlations computational material physics suggests that magnetism is present and plays an important role in the understanding physical behavior of hcp iron under compression.

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Transverse Spin Currents and Torques in Magnetic Multilayers

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A current passing through two ferromagnets separated by a non-magnetic spacer layer exerts a torque on each magnetization whenever the two magnetization directions are not parallel. Modeling this behavior requires three types of calculations. First, quantum mechanical calculations are needed to determine the fate of an electron that scatters from a interface with a ferromagnet. These calculations determine the boundary conditions that are used in the second type of calculation, semiclassical transport calculations. These calculations determine the current and spin current throughout the structure. Together, these two calculations determine the torque on the magnetizations in the structure. Finally, a separation of time scales justifies the third type of calculation, classical simulations of the magnetization dynamics using the calculated torques. Here, we describe our calculations of the first two types.

For coherent interfaces, we have computed the spin-dependent reflection and transmission amplitudes from first-principles. These amplitudes determine the scattering properties for spins, in particular, the fate of the transverse component. The boundary condition that results from this calculation is that the transverse component of the incident spin current is essentially absorbed close to the interface for multilayers of interest. The absorbed spin current corresponds to a torque on the electrons by the ferromagnet with a corresponding reaction torque exerted on the magnetization close to the interface. We have also carried out equivalent calculations for free electron models in order to better understand the processes that contribute to the final result.

Using the boundary condition described above, we have derived and solved (numerically) a matrix Boltzmann equation to determine the transport in a Co/Cu/Co multilayer. This is a semi-classical method which bridges the gap between fully quantum mechanical calculations (valid when the spacer is much thinner than the mean free path) and drift-diffusion calculations (valid when the spacer is much thicker than the mean free path). These calculations highlight the important role played by spin-flip scattering (in the leads or in the magnets), which polarizes the current in the magnets because the majority and minority electrons experience different resistances. When the magnetizations are not collinear, non-collinear spin polarization also develops in the non-magnet. From the spin current and the boundary conditions, we compute the torques on the magnetizations.

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Theory of the Role of Defects in Co-doped TiO_2 Anatase

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With a Curie temperature reported to be well above room temperature, the recently discovered ferromagnetic semiconductor Co-doped TiO_2 anatase is of great interest to the spintronics community. As of yet, there is no consensus as to the specific mechanism that gives rise to long-range magnetic order in this material, nor is the origin of the free carriers, which are experimentally determined to be n-type, understood. To shed light on the situation, we report first principles calculations of the electronic structure of simple and complex defects in TiO_2 anatase in the local density approximation. The resulting impurity levels, carrier type and concentration, as well as the magnetic character are analyzed as a function of experimentally controllable quantities. This analysis suggests possible methods to further enhance the magnetic character of Co-doped TiO_2.

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Ab-initio calculations of anisotropy in spin-fluctuations of Sr_2RuO_4 and hcp-Fe

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The superconducting phase of Sr_2RuO_4 has been conjectured to be due to the formation of Cooper pairs of odd parity (spin triplet) p-wave [1]. 'Anisotropic' anti-ferromagnetic spin fluctuations has been proposed to play a role in stabilising the spin triplet state [2].

Formalism for the anisotropy in the paramagnetic spin susceptibility for multi-atom per unit cell materials is provided. This formulism is based upon a fully relativistic multiple scattering (KKR) theory using Local Density Approximation. Anisotropy is due to relativistic effects are such as spin-orbit interaction. Our calculations of the anisotropy for Sr_2RuO_4 show that anti-ferromagnetic spin fluctuations due to Fermi nesting ($\mathbf{q}_{nest} = (0.35, 0.35, 0)$) are more dominant in the c-axis where as for ferromagnetic spin fluctuations ($\mathbf{q} = 0$) they are stronger in the ab-plane. The temperature dependence of the anisotropy in these spin fluctuations is given. The recent discovery of a superconducting phase in hcp-Fe [3] has lead us to investigate the spin fluctuations. At a pressure of ~ 17 Gpa we find Fermi nesting at $\mathbf{q} = (0.42,0,0)$ leading to anti-ferrmomagnetic spin fluctuations. Calculations of the anisotropy in these spin fluctuations is shown.

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Exchange Couplings in Cuprates and Vanadates from QMC and Ab-Initio Calculations

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Modern quantum Monte Carlo (QMC) algorithm allow the accurate simulation of (unfrustrated or weakly frustrated) quantum magnets on large systems dow to very low temperatures. They can be used on the one hand for the theoretical investigation of thermal and quantum phase transitions in magnetic systems. On the other hand, and this will be the topic of my talk, they can be used for quantitative modeling of quantum magnets. One approach, which was successfully used for cuprate and vanadate ladder materials, a reasonable model for the exchange interactions can be guessed from the crystal structure. A fit of simulation results to experimental measurements of the uniform susceptibility or neutron scattering data for the dispersion can then be used to determine the microscopic exchange couplings. In other more complex materials, such as the vanadates CaV_3O_7, CaV_4O_9 or $(VO)_2P_2O_7$, it is no longer possibly to guess the dominant couplings, and aven the determination of the sign of the interaction can be tricky. Here ab-initio LDA+U calculations can determine values for the exchnange couplings. QMC simulations can then be used to compare these ab-initio exchange couplings to experimental measurements and to obtain improved couplings. In frustrated systems, QMC simulations suffer from a severe negative sign problem and can be applied only at temperatures above the largest frustrating interaction. For these systems high temperature series expansions can be used instead.

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Magnetic Anisotropy in Fe Multilayers on Cu Surfaces: Theory and New Experiments

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The newely developed pulsed laser deposition technique enabled experimental groups to prepare thin film samples which are much better quality, much closer to the idealistic models theories do frequently assume. Therefore it is appropriate to revisite calculations regarding the magnetic phase diagram of the much discussed Fe/Cu(100) and Fe/Cu(111) thin film systems. In this talk I will summarize results obrtained earlier and report on new calculations regarding this old topic.

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Spin Wave Instabilities in Magnetic Switching

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One of the central problems in magnetization dynamics is the understanding of magnetic switching on a nanosecond time scale. This is also an important problem in magnetic information storage technology, because the continued increase of hard-disk writing speeds (now approaching the gigahertz range) require that the grains of hard-disk media switch at these speeds; such high-speed switching is not now well understood. In most treatments of this problem it is assumed that the magnetization is uniform or slowly varying; in this case the Landau-Lifshitz equation can be used to compute the evolution of the magnetization. One barrier to switching is the fact that switching is an exothermic process, and there is no obvious way to quickly dissipate the energy released. We have found, both numerically and analytically, that the uniform-magnetization solution is unstable against the creation of spin waves, and that this can provide an energy dissipation mechanism and permit switching.

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Spin-Polarized Ballistic Electron Transport Through an Interface by an Embedded Green-Function Approach

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We present an efficient method for calculating the conductance of ballistic electrons through magnetic interfaces from first-principles using the embedding approach of Inglesfield [1]. In our method the Landauer-Buttiker formula [2] for ballistic transport is expressed in terms of two quantities that are available in the embedded Green-function formalism without additional calculations. One is the embedding potential of bulk crystals on both sides of the interface and the other is the Green function in the interface region. The embedding formulation was implemented within the framework of the full-potential linearized augmented plane wave (FLAPW) method using the FLEUR code [3]. The actual implementation is discussed in detail. We will present calculations for magnetic multilayer structures used in giant magneto- resistance (GMR) and tunneling magneto-resistance (TMR) devices. In order to check the accuracy, and to allow a comparison with previous calculations we have chosen as an example of a GMR system, the Cu/Co/Cu(100) sandwich structure which is a model system in magneto- electronics and intensively investigated before. As a second application we present the investigation of the spin-resolved electronic tunneling through a Fe/MgO/Fe TMR junction.

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Advanced Tetrahedrally-Bonded Magnetic Semiconductors for Spintronic Applications

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Recent developments of magnetic semiconductors suggest the possibility of harnessing the spin of the electron – in addition to its charge – for future semiconductor devices. Chalcopyrites, which are genealogically related to the zinc-blende structure, provide promising magnetic semiconductor candidates for future applications for which the Curie temperature is limited in Mn doped III-V semiconductors. From highly precise FLAPW calculations, we found that: i) Mn doped II-Ge-V2 (when Mn goes to II sites) chalcopyrites are AFM favored and will undergo a phase transition to FM state when n-type S doping is introduced. As a result, the magnetic moments may be tuned by the impurity concentrations, which will be a great boon for technological applications. ii) A new class of half-metallic ferromagnetic semiconductors in Mn doped I-III-VI2 chalcopyrites is predicted. The estimated Curie temperature is proportional to the hole concentration. It is exciting for our theoretical prediction that a recent experiment confirmed that CuGa1-xMnxTe2 shows strong ferromagnetic coupling with a Tc of about 240K.

Most recently, to understand the origin of the ferromagnetism in Mn doped Ge, we investigated the electronic and magnetic properties of MnxGe1-x (x=0.031) as a function of the Mn positions in a 64 atom supercell. The FM aligned Mn with distance of sqrt2*a has the lowest energy, followed by several energetically competitive FM and AFM aligned Mn configurations. This explains the existence of "inactive" Mn magnetic moments in experiments, while the theoretical magnetic moment is 4 muB per Mn for the FM states. The exchange interaction between Mn ions oscillates as a function of the distance between them, and obeys the RKKY analytic formula. Our theoretical results for x=0.047 and 0.063 cases are also explained with the same RKKY formula. In addition, the estimated highest Curie temperature, around 134 K, is in good agreement with experiment.

In collaboration with Tatsuya Shishido, Silvia Picozzi, Alessandra Continenza, Wen-Tong Geng. Supported by the NSF MRSEC Program.

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